

4-Hexylresorcinol
136-77-6 | DTXSID1020699

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 80.7 °C

Global applicability domain: Inside

Local applicability domain index: 8.24e-01

Confidence level: 5.70e-01

Nearest Neighbors from the Training Set

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4-Hexylresorcinol

Measured: 68.0

Predicted: 80.7

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1,3-Benzenediol, 4-pentyl- (9CI)

Measured: 72.5

Predicted: 79.2

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tert-Butylhydroquinone

Measured: 128

Predicted: 101

Image not found

4-Propylresorcinol

Measured: 82.5

Predicted: 124

Image not found

3-Cyclohexene-1,1-dimethanol

Measured: 88.5

Predicted: 97.0